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# USE OF PETROLEUM-BASED CORRELATIONS AND ESTIMATION METHODS FOR SYNTHETIC FUELS

A.C. Antoine  
*Lewis Research Center*  
*Cleveland, Ohio*

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# USE OF PETROLEUM-BASED CORRELATIONS AND ESTIMATION METHODS FOR SYNTHETIC FUELS

by A. C. Antoine

National Aeronautics and Space Administration  
Lewis Research Center  
Cleveland, Ohio 44135

## SUMMARY

E-485 | Correlations of hydrogen content with aromatics content, heat of combustion, and smoke point are derived for some synthetic fuels prepared from oil shale and coal syncrudes. These correlations are compared with correlations that have been derived for petroleum fuels. The results show that the hydrogen content-aromatics content correlation derived for petroleum fuels can be used for the shale-derived fuels. The coal-derived fuels do not fit the correlation as well, and a separate correlation is recommended. In regard to the correlations with heat of combustion and smoke point, the results are comparable to some found for petroleum fuels.

Calculated values of hydrogen content and heat of combustion are obtained by use of ASTM estimation methods, to assess their applicability to the synthetic fuels. Comparison of the measured and calculated values of hydrogen content show a bias in the equation that exceeds the critical statistics value. However, the magnitude is not as great as the biases in other equations suggested (ref. 7) for use with petroleum fuels. A decided bias is also found in using the calculation method for determining the heat of combustion to the extent that, if the measured values are accurate, its use would be precluded.

Comparison is made of the measured hydrogen content by the standard ASTM combustion method with that by a nuclear magnetic resonance (NMR) method (recently adopted as ASTM D3701). A decided bias was found, with most NMR values higher than the values from the combustion method. The comparison of the calculated and measured NMR hydrogen contents show a difference similar to that found with petroleum fuels.

## INTRODUCTION

The purpose of this report is to compare hydrogen content correlations of some synthetic fuels with correlations that have been derived from petroleum fuels, and to assess the applicability, to these synthetic fuels, of estimation methods for obtaining hydrogen content and heat of combustion. In the report, hydrogen content correlations with aromatics content, heat of combustion, and smoke point are determined. These correlations, determined from fuel samples derived from oil shale and coal syncrudes, are compared with those determined using petroleum-based fuels (refs. 1-2).

In determining properties of petroleum fuels, long experience and extensive data have led to the development of methods for estimating the hydrogen content and the heat of combustion. These methods make use of the volatility, density, and aromatic(s) content of the fuel in the estimation. For a number of synthetic fuels these properties may vary from those of con-

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ventional jet fuels, showing lower volatility, higher specific gravity, and higher aromatics content. In this report, a comparison is made of the measured hydrogen content of a number of synthetic fuels (measured by ASTM D1018, Test for Hydrogen in Petroleum Fractions) with that of a calculated hydrogen content (calculated by ASTM D3343, Estimation of Hydrogen Content of Aviation Fuels). In addition, the measured heat of combustion (by ASTM D2382, Heat of Combustion of Hydrocarbon Fuels by Bomb Calorimeter (High Precision Method)), is compared with calculated results (by ASTM D3338, Estimation of Heat of Combustion of Fuels). Finally, comparison is made of the measured hydrogen content itself, comparing the results of the standard method, ASTM D1018, with those obtained by nuclear magnetic resonance, using the method newly adopted as ASTM D3701, Hydrogen Content of Aviation Turbine Fuels by Low Resolution Nuclear Magnetic Resonance Spectrometry.

## FUELS

The fuels examined in this work were those prepared from TOSCO shale oil, H-Coal and COED coal syncrudes by the Atlantic-Richfield Company (ARCO) under a NASA contract (ref. 3). Thirty-two jet fuel samples of varying properties were produced by processes commonly in use in petroleum processing, distillation, hydrogenation and catalytic hydrocracking. The processing conditions were those required to meet two levels of specifications regarding aromatic, hydrogen, sulfur, and nitrogen contents at two yield levels. Each process stream was split by distillation to give four distillation ranges. The volatility specifications and properties of the fuels produced are given in table I. The fuels had specifications approximating those of (1) JP-4 (Jet B) with a 561K end point, (2) JP-5 (Jet A) with a 561K end point, (3) a broad specification fuel incorporating the volatility of a JP-4 and the end point of a diesel No. 2, at 616K, and (4) Diesel No. 2 with a 616K end point. All the physical and chemical tests required for aircraft turbine fuels were reported by ARCO for the 32 fuels using standard ASTM methods (ref. 4). Sixteen of these fuels were from a TOSCO shale oil syncrude, 8 from an H-coal syncrude, and 8 from a COED (coal-derived) syncrude. In table II are values for the heat of combustion, and for hydrogen content determined by nuclear magnetic resonance (NMR). The latter values were determined by the Wright-Patterson Air Force Laboratory, using a method recently adopted as ASTM D3701, Hydrogen Content of Aviation Turbine Fuels by Low Resolution Nuclear Magnetic Resonance Spectrometry. The heats of combustion were determined by the Lewis Research Center using ASTM D2382.

## RESULTS AND DISCUSSION

### Aromatics Content-Hydrogen Content Correlations

In considering hydrogen content as an estimate of other fuel properties, one of the prime considerations has been to correlate hydrogen content with aromatics content. It is expected, though, that exact correlations with aromatics content cannot be found since the hydrogen content varies with molecular weight, as well as being a function of the molecular structure. Thus, the correlations would be dependent on the mix in the fuel of normal paraffins, which are rich in hydrogen, unalkylated aromatics, which are hydrogen poor, and intermediate species, such as alkylated and partially hydrogenated aromatics. Fuels derived from shale oil syncrudes have been shown to be more like petroleum fuels than are fuels derived from coal

syn-crudes. Coal liquids in general are high in aromatics and low in paraffins. Further, typical hydroprocessing catalysts convert the aromatics and low in paraffins. Further, typical hydroprocessing catalysts convert the aromatics to naphthenes without substantial cracking to produce paraffins. Further, typical hydroprocessing catalysts convert the aromatics to naphthenes without substantial cracking to produce paraffins. In figure 1 is the data and the straight line fitted to the data (by the method of least squares) for the 32 samples examined in this work. The equation for the straight line is  $Y = -12.013X + 179.03$ , S.D. = 0.380, where  $Y$  is the aromatics content and  $X$  is the hydrogen content, determined by the ASTM D1018 method. Since the data seemed to segregate itself, it was deemed proper to fit two lines to the data. This was done and the results shown in figure 2, with one curve for the coal fuels and one for the shale fuels. The slopes of the lines are slightly different, and the S.D. of each is less than that of the combined data shown in figure 1.

An illustration of a correlation developed with petroleum fuels is found in reference 1, where data for 50 fuels are given. The hydrogen content ranged from 12.3 to 15.0, including JP-4, kerosene, and diesel fuels. Data from 23 of those fuels was used to derive the equation, and the straight line is shown in figure 3. The equation is  $Y = -14.243X + 214.99$ , with a S.D. = 0.199. The standard error of estimate in  $Y$  is also shown. For comparison the synthetic fuel data is plotted also in figure 3, and it can be seen that quite a number of shale fuels fit within one standard error of estimate of the curve from the petroleum fuels. The fuels from the coal syn-crudes did not. A plausible explanation is that even when low in aromatics, the coal liquids are expected to have higher concentrations of saturated ring compounds such as monocycloparaffins and di-cycloparaffins (decalins) than typical petroleum fuels. It should be noted also, seen clearly in figure 2, that for a given aromatics level, the shale fuels have a hydrogen content about 0.6 of a percent higher than the coal fuels. This result is probably due, in part, to a substantially higher paraffin content in the shale fuels. A similar result was reported in reference 5 in comparing shale fuels to coal and petroleum fuels. It appears that separate aromatics content-hydrogen content correlations should be made for shale oil and coal derived fuels.

#### Heat of Combustion - Hydrogen Content Correlations

The heat of combustion of a fuel is directly related to the hydrogen content of the fuel. The higher the hydrogen content, the higher the heat of combustion will be. Present jet fuel specifications are not given in terms of hydrogen content, but by specifying a minimum allowable net heat of combustion, a minimum hydrogen content is indirectly specified. Further, since current jet fuel specifications limit the percentages of olefins and aromatics allowed, the minimum hydrogen content of the fuel is also controlled. Attempts have been made to correlate weight percent hydrogen with the net heat of combustion over a range of hydrogen content that includes that of interest, about 12.5 to 15.0. For the fuels examined here, the shale hydrogen content ranged only from 13.37 to 13.98 weight percent, while the coal values ranged from 12.47 to 13.73. The values for the heat of combustion as a function of hydrogen content of each of 30 synfuels are plotted in figure 4. The curve generated from the synfuel data by the method of

least squares is also shown. The equation for the curve is  $Y = 565.66X + 34,885$ , S.D. = 0.0144. The correlation coefficient is 0.373.

In reference 2 are petroleum data from several sources which show quite good agreement over the range from 12.5 to 15.0 weight percent hydrogen. (The sets of data used to make the correlations ranged from 7 to 134, and the range in correlation coefficients was from 0.525 to 0.991, not respectively). An average of the correlation curves over that range was taken in reference 2 and values were selected as being a reasonable "best estimate" for correlating hydrogen content with the net heat of combustion. We have taken those values and drawn a curve which is also shown in figure 4.

The values for the "best estimate" curve lie about  $1\frac{1}{4}$  percent above the generated line, but lie within one standard error of estimate in the values for the heat of combustion. In assessing the accuracy of the measured heat of combustion values, repeated measurements of the heat of combustion of two pure hydrocarbons, dodecane and decahydronaphthalene, were made. For both compounds the measured value was about 1 percent lower than the handbook value. This suggests that all of the measured values may be low by about 1 percent. If this is true the generated line would be closer to the "best estimate", but the correlation would still be poor.

#### Smoke Point - Hydrogen Content Correlations

Smoke points have, for some time, been used as a measure of a fuel's expected combustion performance. Limits have been placed on smoke points as a means of specifying and controlling the fuel's combustion properties. A number of correlations with hydrogen have been made (ref. 2) with some disagreement among the correlation curves. Straight-line curves and other fits involving second order equations have been made to describe hydrogen content-smoke point relations. The data from the synthetic fuels in this study are plotted in figure 5. A straight-line curve was fitted to the data by the method of least squares, and is shown as the solid line in the figure. The equation is  $Y = 8.513X - 93.285$ , S.D. = 0.087. The correlation coefficient is 0.896. In the figure also is a dashed line which represents the preferred correlation as determined in reference 2. This curve was based on data reflecting the properties of petroleum jet fuels. It appears that it could be useful for synthetic fuels with smoke points above 20. An example of a curve from a second order equation is also shown in the figure as a broken line. This curve is from reference 5 and was derived from JP-5 type fuels from oil shale, coal, and tar sands as well as petroleum-based fuels. The fit of this curve to the data is reasonable, particularly at hydrogen contents above 13.20. Other correlations with petroleum fuels of widely varying composition and some pure hydrocarbons have been described (ref. 2), with both low and high correlation coefficients. The curve derived from the data in this report is of somewhat different slope from the preferred correlation suggested in reference 2, but comparable to other correlations found for smoke point and hydrogen content.

#### Estimation Method for Hydrogen Content

The ASTM method D3343, Estimation of Hydrogen Content of Aviation Fuels, is empirical and applicable to liquid hydrocarbon fuels that conform to the requirements of specifications for aviation gasolines or aircraft

turbine and jet engine fuels. The use of this correlation may be applicable to other hydrocarbon distillates similar to aviation fuels, but only limited data on nonaviation fuels were included in the correlation. The correlation has been established between the hydrogen content and its distillation range, API gravity, and aromatic content. The equation requires the average of the 10, 50, and 90 percent distillation data (using method D86, Distillation of Petroleum Products). These values were obtained from reference 6. Distillation data can also be obtained by method D2887, Boiling Range Distribution of Petroleum Fractions by Gas Chromatography, and this method is under study for use in describing fuels. The 10, 50, and 90 percent distillation data needed for the estimation method can be calculated from the D2887 data, and those values were also obtained from reference 6. The results from using both sets of data for H-content are given in table III. A comparison of the measured and calculated values are shown in figure 6(a) and (b). To further compare the values, an analysis of the difference in measured and calculated hydrogen content was made and the results are given in table IV. Given are the average difference between the measured and calculated values, the standard deviation of the average difference, and the  $\tau$  statistic. The  $\tau$  statistic is computed by using the average difference and the standard deviation, and is used to test for equation bias. The results obtained indicate a bias in the equations (the  $\tau$  statistic exceeds the critical value of 2.05, where  $\tau$  values are for two-tailed significance tests at the 95 percent confidence interval with N-1 degrees of freedom). It should be noted, however, that other equations suggested for calculating hydrogen content, in reference 7, shows biases of this magnitude. It can be expected, thus, that with data from synthetic fuels included in the correlation, the estimation method can be made useful.

#### Estimation Method for Heat of Combustion

The method for estimating the heat of combustion of aviation fuels (ASTM D3338) is purely empirical and applicable to liquid hydrocarbon fuels that conform to the specifications for aviation gasolines, aircraft turbine, and jet engine fuels of certain grades. It is not intended as a substitute for experimental measurements of heat of combustion, but can find use where an estimate is satisfactory. To make the calculation, the specific gravity, aromatic content, and average volatility of the fuel is needed. Further, the sulfur content, given in table I, is used in calculating the net heat of combustion on a sulfur-free basis. The results of the determination are given in table V. A comparison of the values from the measured method and the calculated method is shown in figure 7(a) and (b), again using distillation data from D86 and D2887. The results of an analysis of the differences in the measured and calculated heats of combustion are given in table VI. The  $\tau$  value bears out the visual evidence that there is a decided bias in the equation. The correlation equations were developed using 241 fuels, 169 of which were aviation fuels (or similar thereto). The remaining 72 fuels were pure hydrocarbons. The equation as developed should give calculated values within 105 J/g of measured heating values for aviation fuels, or 347 J/g when pure hydrocarbon fuels are included. It should be remembered, as noted before, that the measured values may all be low by about 1 percent, which if true would substantially improve the agreement. Nevertheless, the great disparity found with the synthetic fuels suggests that such fuels will have to be included in the group of calibrating fuels for the calculating method,

as well as validating the accuracy of the measured combustion method with these fuels.

#### NMR Measurements and Comparisons

The results from the measurements of the hydrogen content by an NMR spectrometer are given in table II. A comparison of the values from D1018 and the magnetic resonance technique is shown in figure 8. An analysis of the differences is given in table VII. The results show a decided bias in the NMR readings, with most NMR values reading higher than the values from the combustion method. This is unexpected in that previous work (ref. 8) with aviation turbine fuels had shown good agreement in determinations by the combustion technique and by the low resolution NMR method. The errors observed there appeared to be random, with no bias toward fuels of a particular type or composition being discernible.

In another study, reference 9, a comparison is made of calculated (D3343) and measured (NMR) hydrogen contents of (236) samples of petroleum Jet A fuels. The hydrogen content as measured by NMR had a mean value 0.16% (abs.) higher than the mean from the calculated method. Looking at a similar comparison from the fuels (8JP-5 type fuels) from this work showed the following:

	ASTM D3343(D86)	ASTM D3343(D2887)	NMR
Mean value	13.47	13.45	13.58

Thus a similar difference is noted with NMR readings averaging about 0.12% (abs.) higher than the calculated values. In this respect the results for the synthetic fuels are similar to those for the petroleum fuels.

#### SUMMARY OF RESULTS

1. The shale-derived fuels examined in this work can be correlated by hydrogen content and aromatic content relationships used for petroleum fuels. The coal-derived fuels cannot, as easily. It is suggested from the results that a separate correlation for coal fuels be made.

2. The correlation of hydrogen content with heat of combustion is similar to that of the petroleum fuels, with the measured values of heat of combustion about  $1\frac{1}{4}$  percent lower than those of the "best estimate" petroleum curve suggested in reference 2. The correlation though is poorer than most found with petroleum fuels, and, also, there is evidence that the measured heat values may be low by about 1 percent.

3. The correlation of smoke point with hydrogen content is comparable to some that have been derived for petroleum fuels, though of different slope from the "preferred" correlation suggested in reference 2.

4. Comparison of the measured (ASTM D1018) and calculated (ASTM D3343) hydrogen content showed a bias in the equation that exceeded the critical value. However, the magnitude was not as great as other equations suggested in reference 7 for use with petroleum fuels.

5. A decided bias was also found in using the calculation method (ASTM D3338) for determining the heat of combustion, to the extent that if the measured values are accurate its use would be precluded.

6. The comparison of the D1018 measured values with those from the NMR method showed a decided bias in the NMR readings. The comparison of the calculated (D3343) and measured NMR hydrogen contents showed a difference similar to that found with petroleum fuels.

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TABLE 1. - FUEL PROPERTIES

Fuel no.		Flash point, K	REID vapor pressure, kN/m <sup>2</sup>	Specific gravity kg/m <sup>3</sup>	Smoke point, mm	Aromatics, vol. %	Naphthalenes, percent	Olefins, vol. %	Hydrogen, wt. %, ASTM D1018	Sulfur, wt. %
1	Shale		0.34	794.5	22	19.0	0.5	1.0	13.73	0.0006
2			1.1	791.4	26	13.5	.2	.9	13.76	.0002
3	IBP-561K		6.9	787.4	25	13.7	.33	.8	13.70	.0005
4			7.6	787.4	27	11.4	.17	.8	13.98	.0005
5	Coal, IBP-561K H-coal		1.1	841.3	16	26.3	0.27	1.2	12.79	0.0001
6			3.1	831.4	25	5.5	.055	.9	13.73	.0001
7	COED		7.2	827.0	19	20.1	.31	.5	13.24	.0001
8			5.8	816.5	27	5.4	.11	.5	13.69	.0001
9	Shale	311		806.8	21	22.2	0.5	1.1	13.68	0.0006
10		312		802.2	24	17.1	.2	1.2	13.95	.0001
11	394-561K	312		805.4	22	17.9	.42	1.3	13.80	.0006
12		309		803.5	25	13.2	.21	1.0	13.95	.0002
13	Coal, 394-561K H-coal	309		856.5	15	30.9	0.31	1.4	12.64	0.0001
14		314		846.8	24	5.8	.065	1.0	13.31	<.0001
15	COED	313		849.3	16	25.2	.38	.8	12.96	.0001
16		314		836.8	24	7.2	.13	.9	13.63	.0001

TABLE I. - Concluded.

Fuel no.		Flash point, K	REID vapor pressure, kN/m <sup>2</sup>	Specific gravity kg/m <sup>3</sup>	Smoke point, mm	Aromatics, vol. %	Naphthalenes, percent	Olefins, vol. %	Hydrogen, wt. % ASTM D1018	Sulfur, wt. %
17	Shale	315		817.0	20	25.9	1.2	0.8	13.66	0.0044
18		312		808.1	26	17.4	.4	1.0	13.86	.0003
19	394-616K	314		814.6	20	20.3	.93	.9	13.37	.0012
20		312		810.0	25	15.4	.35	1.0	13.95	.0002
21	Coal, 394-616K H-Coal	312		865.4	15	33.8	0.66	1.8	12.47	0.0004
22		312		848.8	21	6.7	.077	1.4	13.26	.0005
23	COED	319		858.6	14	28.5	.86	1.2	12.88	.0001
24		313		845.8	20	11.6	.62	1.1	13.44	.0003
25	Shale		1.1	804.0	21	21.9	1.0	1.1	13.64	0.0010
26			2.8	797.7	26	13.7	.4	.8	13.82	.0009
27	IBP-616K		7.6	797.2	23	15.7	.75	.8	13.82	.0014
28			8.6	793.6	26	12.1	.3	.6	13.98	.0011
29	Coal, IBP-616K H-Coal		1.4	849.3	14	29.7	0.54	1.2	12.73	0.0004
30			1.7	833.8	24	5.9	.064	1.3	13.56	.0005
31	COED		5.8	835.8	16	22.4	.68	.6	13.07	.0003
32			5.8	825.5	20	9.3	.49	.7	13.53	.0003

TABLE II. - FUEL PROPERTIES

Fuel no.		Heat of combustion, J/g	Hydrogen, wt.%
		ASTM D2382	NMR
1	Shale	42456	13.96
2		42963	14.29
3		42873	14.15
4		42735	14.27
5	H-Coal	41874	12.84
6	COED	41772	13.81
7		42938	13.32
8		42653	13.89
9	Shale	-----	13.78
10		42063	14.18
11		43100	13.99
12		42767	14.05
13	H-Coal	41870	12.47
14	COED	42187	13.86
15		42191	13.03
16		-----	13.27
17	Shale	45084	13.69
18		41856	14.13
19		43294	13.93
20		43114	14.01
21	H-Coal	42238	12.50
22	COED	42032	13.61
23		41262	12.90
24		42793	13.53
25	Shale	42440	13.96
26		42402	14.24
27		42350	14.08
28		42460	14.26
29	H-Coal	41959	12.74
30	COED	42645	13.79
31		42358	13.20
32		42484	13.71

TABLE III. - HYDROGEN, WT. PERCENT

Fuel no.		ASTM D1018	ASTM D3343 (D86)	ASTM D3343 (D2887)
1	Shale	13.73	13.81	13.82
2		13.76	14.08	14.10
3		13.70	14.09	14.10
4		13.98	14.22	14.19
5	H-Coal	12.79	12.83	12.79
6	COED	13.73	13.66	13.64
7		13.24	13.26	13.23
8		13.69	13.92	13.92
9	Shale	13.68	13.60	13.58
10		13.95	13.85	13.85
11		13.80	13.76	13.76
12		13.95	13.97	13.95
13	H-Coal	12.64	12.54	12.53
14	COED	13.31	13.48	13.45
15		12.96	12.92	12.88
16		13.63	13.61	13.59
17	Shale	13.66	-----	-----
18		13.86	13.88	13.89
19		13.37	13.68	13.69
20		13.95	13.91	13.91
21	H-Coal	12.47	-----	12.48
22		13.26	-----	13.45
23	COED	12.88	-----	12.83
24		13.44	13.45	13.43
25	Shale	13.64	13.73	13.81
26		13.82	14.09	14.13
27		13.82	13.98	14.02
28		13.98	14.18	14.20
29	H-Coal	12.73	12.70	12.72
30		13.56	13.66	13.65
31	COED	13.07	13.17	13.19
32		13.53	13.72	13.73

TABLE IV. - ANALYSIS OF DIFFERENCES IN HYDROGEN  
CONTENT AS MEASURED BY METHOD D1018 AND  
CALCULATED BY METHOD D3343 (USING TWO  
SETS OF DISTILLATION DATA)

Statistic	D1018-D3343 differences	
	Distillation data (D3343)	
	D86	D2887
Average difference, $\bar{\Delta}$	0.087	0.084
Standard deviation of average difference, $S_{\bar{\Delta}}$	.140	.148
$\tau$	3.29	3.16

TABLE V. - HEAT OF COMBUSTION, NET, J/g

Sample	Measured, ASTM D2382	Calculated	
		ASTM D3338 (D2887)	ASTM D3338 (D86)
1	42456	43272	43267
2	42963	43423	43408
3	42873	43415	43411
4	42735	43463	43481
5	41874	42646	42674
6	41772	43079	43099
7	42938	42900	42919
8	42653	43258	43258
9	-----	43145	-----
10	42063	43291	43291
11	43100	43233	43238
12	42767	43328	43342
13	41870	42500	42509
14	42187	42967	42989
15	42191	42697	42724
16	-----	43065	43082
17	45084	-----	-----
18	41856	43327	43322
19	43294	43214	43210
20	43114	43327	43327
21	42238	42474	-----
22	42032	42974	-----
23	41262	42676	-----
24	42793	42987	43001
25	42440	43303	43249
26	42402	43456	43428
27	42350	43393	43364
28	42460	43486	43468
29	41959	42617	42607
30	42645	43096	43103
31	42358	42888	42879
32	42484	43168	43160

TABLE VI. - ANALYSIS OF DIFFERENCES IN HEAT  
OF COMBUSTION AS MEASURED BY METHOD D2382  
AND CALCULATED BY METHOD D3338 (USING  
TWO SETS OF DISTILLATION DATA)

Statistic	D2382-D3338 differences	
	Distillation data (D3338)	
	D86	D2887
Average difference, $\bar{\Delta}$ , J/g	659	680
$\tau$	8.70	9.01

TABLE VII. - ANALYSIS OF DIFFERENCES IN  
HYDROGEN CONTENT AS MEASURED BY  
METHOD D1018 AND BY NMR

Statistic	D1018-NMR differences
Average difference, $\bar{\Delta}$	0.183
Standard deviation of average difference, $S_{\bar{\Delta}}$	.199
$\tau$	5.20

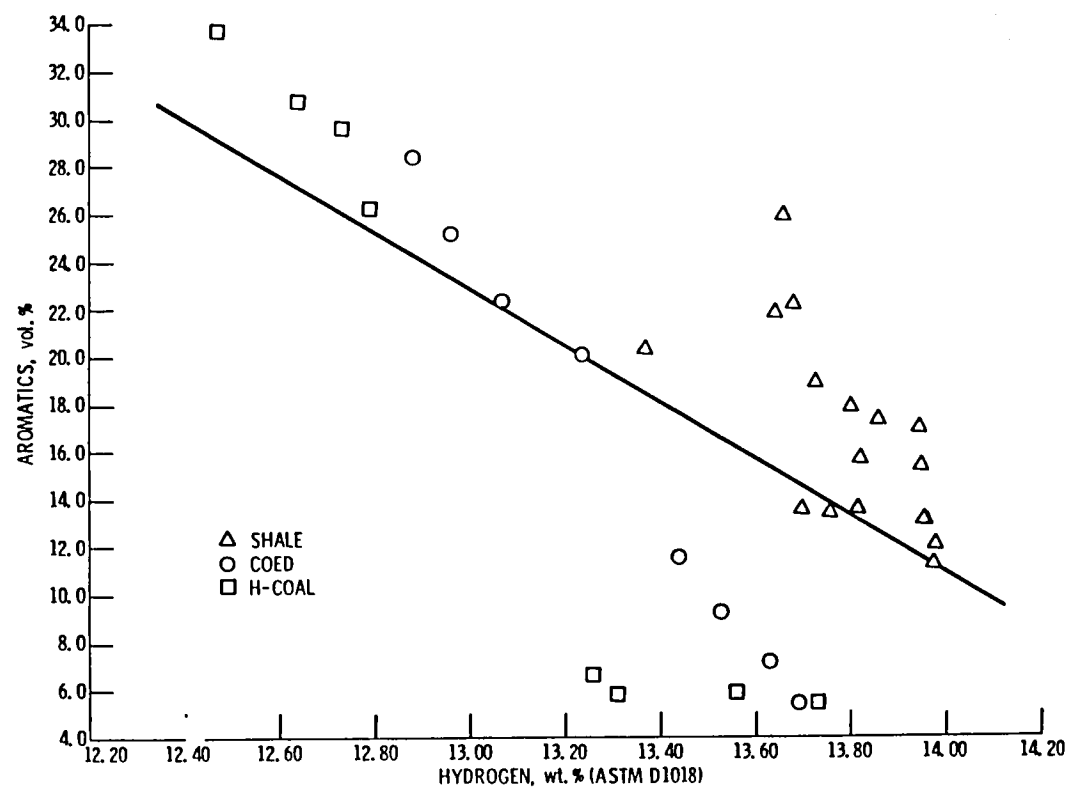


Figure 1. - Aromatic content - percent hydrogen correlation for 32 synthetic fuels.

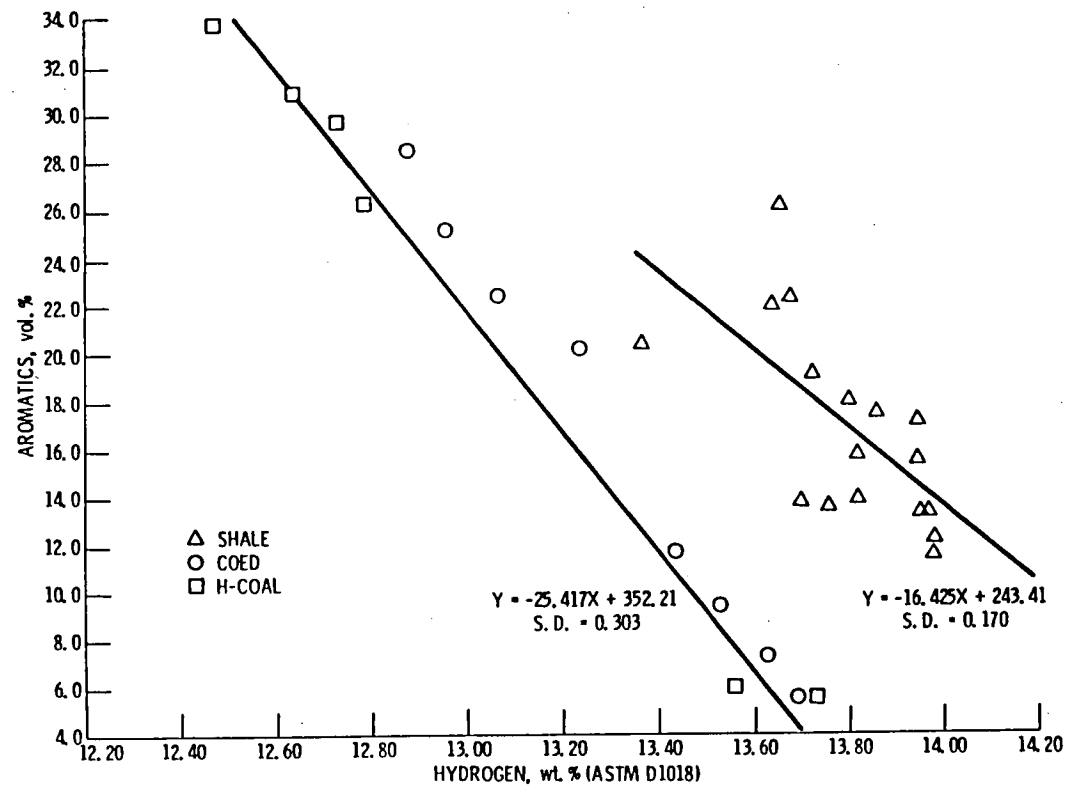
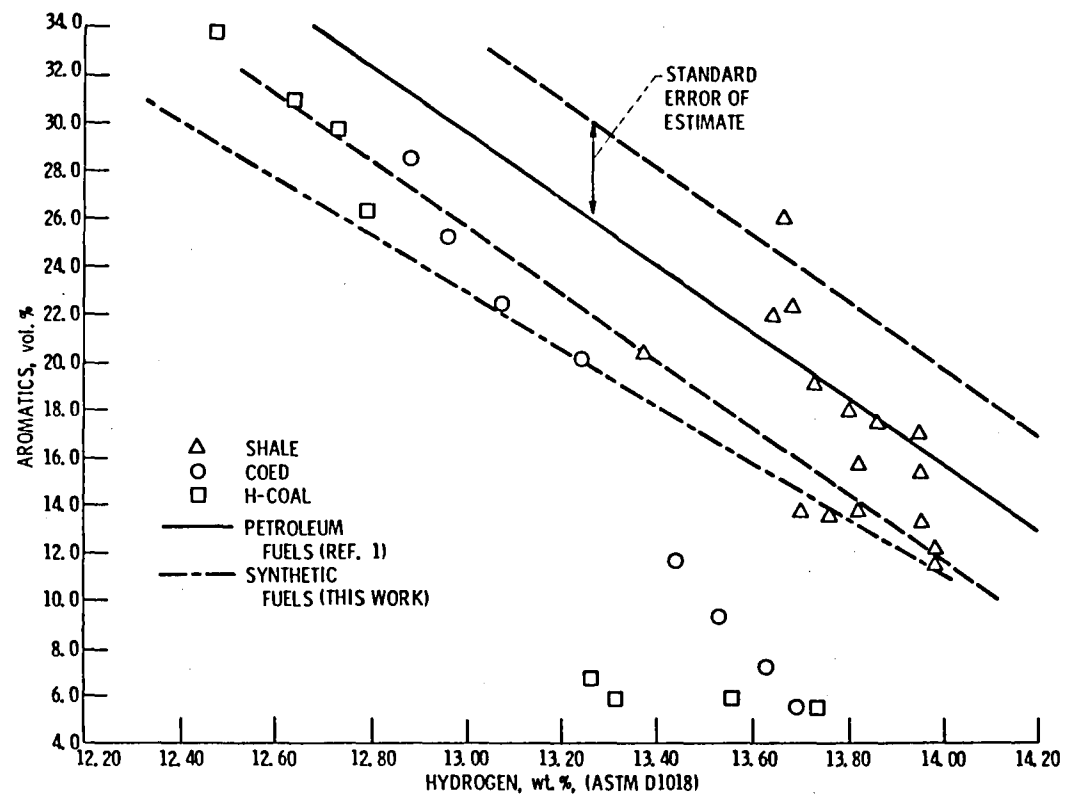


Figure 2. - Aromatic content - percent hydrogen correlations for coal-derived and shale-derived fuels.





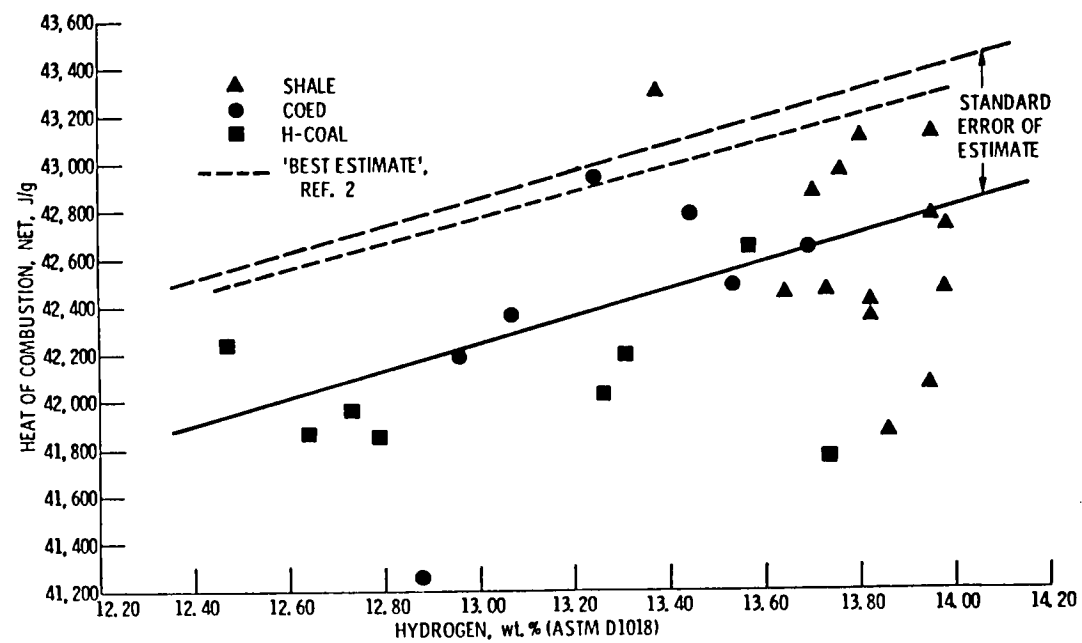


Figure 4 - Correlation of measured (ASTM D2382) net heat combustion and percent hydrogen for synthetic fuels. Comparison with petroleum 'best estimate' correlation.

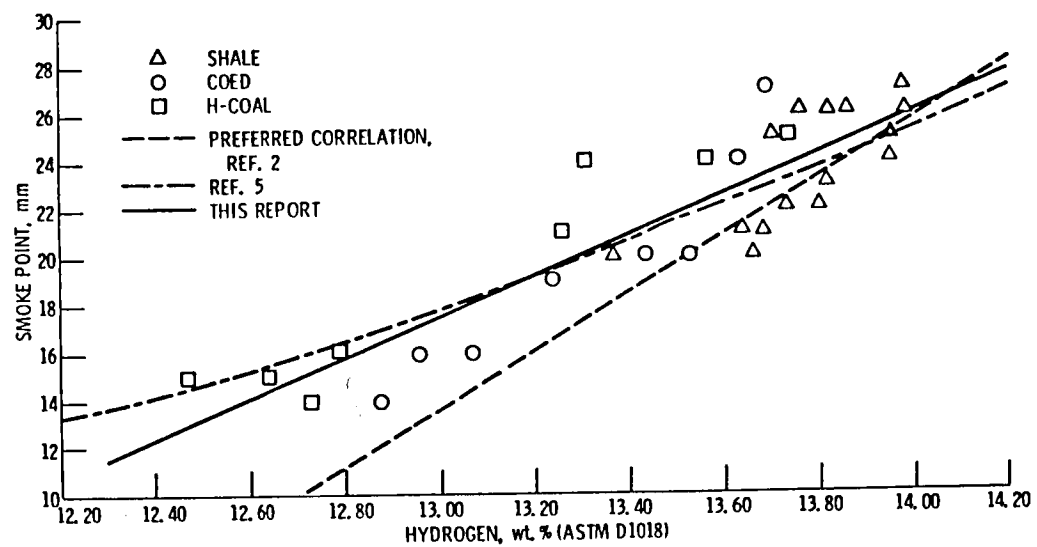
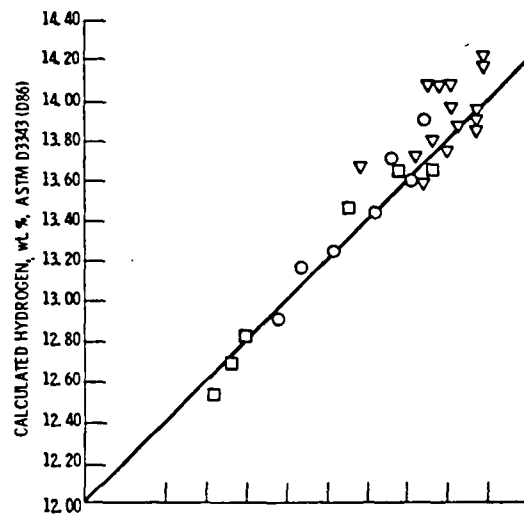
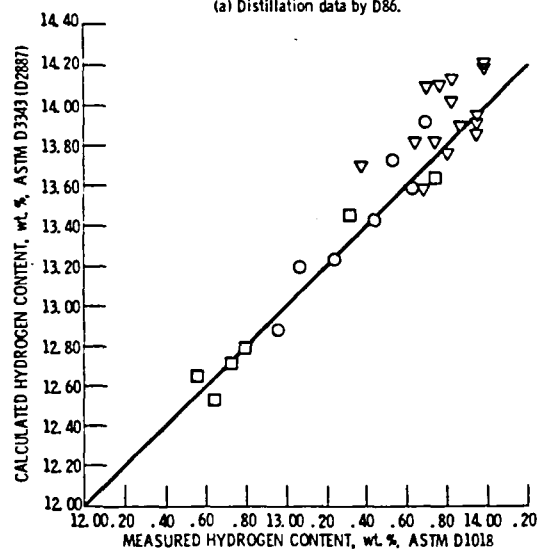


Figure 5: - Smoke point - percent hydrogen correlations - synthetic and petroleum based.

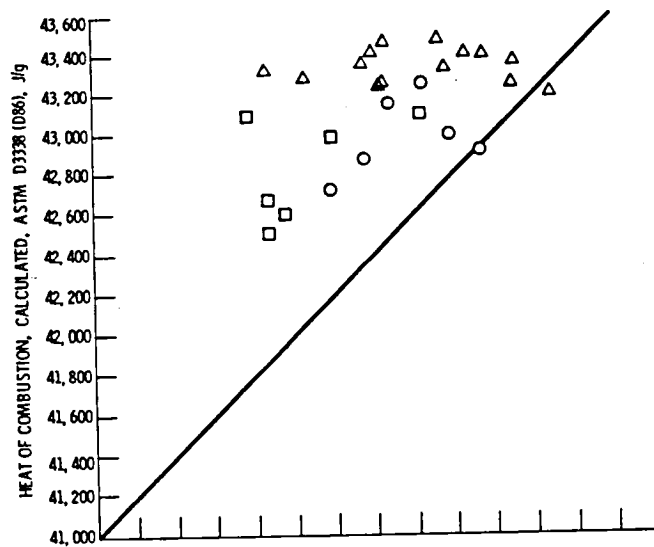


(a) Distillation data by D86.

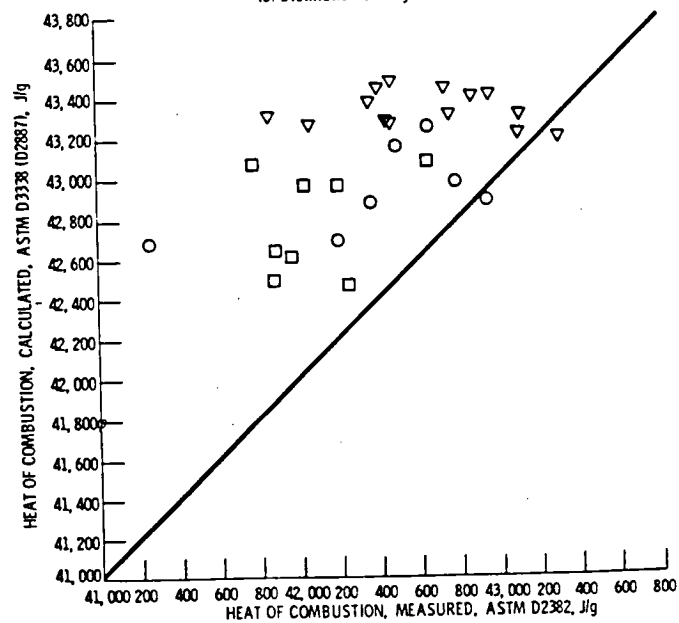


(b) Distillation data by D2887.

Figure 6. - Comparison of hydrogen content measured by ASTM D1018 and calculated by ASTM D3343.



(a) Distillation data by ASTM D86.



(b) Distillation data by D2887.

Figure 7. - Comparison of heat of combustion measured by ASTM D2382 and calculated by ASTM D3338.

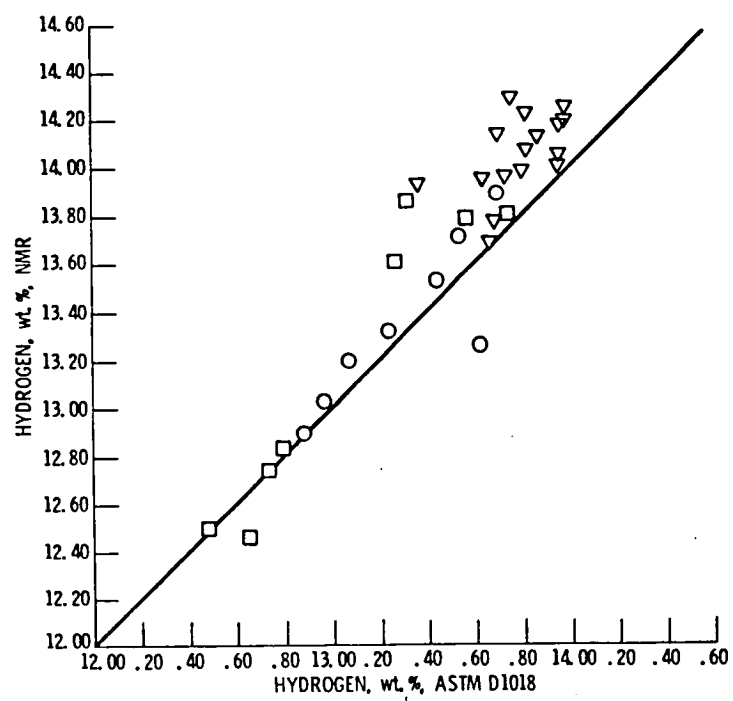


Figure 8. - Comparison of hydrogen content measured by ASTM D1018 and by NMR.

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16. Abstract <p>Correlations of hydrogen content with aromatics content, heat of combustion, and smoke point are derived for some synthetic fuels prepared from oil shale and coal syncrudes. Comparing the results of the aromatics content with correlations that have been derived for petroleum fuels shows that the shale-derived fuels fit the petroleum-based correlations, but the coal-derived fuels do not. The correlations derived for heat of combustion and smoke point are comparable to some found for petroleum-based correlations. Calculated values of hydrogen content and of heat of combustion are obtained for the synthetic fuels by use of ASTM estimation methods. Comparisons of the measured and calculated values show biases in the equations that exceed the critical statistics values. Comparison of the measured hydrogen content by the standard ASTM combustion method with that by a nuclear magnetic resonance (NMR) method shows a decided bias. The comparison of the calculated and measured NMR hydrogen contents show a difference similar to that found with petroleum fuels.</p>			
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